

Randomness-Driven Quantum Phase Transition in Bond-Alternating Haldane Chain

Takayuki ARAKAWA*, Synge TODO^{1†} and Hajime TAKAYAMA*Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan*¹*Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan*

(Received October 29, 2004)

The effect of bond randomness on the spin-gapped ground state of the spin-1 bond-alternating antiferromagnetic Heisenberg chain is discussed. By using the loop cluster quantum Monte Carlo method, we investigate the stability of topological order in terms of the recently proposed twist order parameter [M. Nakamura and S. Todo: Phys. Rev. Lett. **89** (2002) 077204]. It is observed that the dimer phases as well as the Haldane phase of the spin-1 Heisenberg chain are robust against a weak randomness, though the valence-bond-solid-like topological order in the latter phase is destroyed by introducing a disorder stronger than the critical value.

KEYWORDS: Haldane chain, bond randomness, quantum phase transitions, random-singlet phase, quantum Monte Carlo, loop algorithm, topological order, twist order parameter

Disorder effects on low-dimensional quantum magnets have been investigated extensively in recent theoretical studies. In particular, impurity effects on spin-gapped Heisenberg antiferromagnets¹ have aroused much interest in relation to the impurity-induced antiferromagnetic (AF) long-range order observed experimentally in real materials.² It has been established by recent numerical simulations^{3,4} that in two dimensions or higher, there are two classes of disorder, that affect spin-gapped states in essentially different ways. Site dilution and bond dilution are representatives of each class. The former induces localized moments around impurity sites. There exist strong correlations between such effective spins retaining the staggeredness with respect to the original lattice, and therefore the AF long-range order emerges by an infinitesimal concentration of dilution. In the bond-dilution case, on the other hand, localized moments are always induced in pairs and they form a singlet again by AF interactions through the two- or three-dimensional shortest paths as long as the concentration of bond dilution is smaller than a finite critical value.

In one dimension, since quantum fluctuations are much stronger than those in higher-dimensional systems, novel quantum critical phenomena are observed under disorder at the magnitude of coupling constants (bond randomness). Theoretically, the decimation renormalization group (DRG) approaches have achieved great success in predicting rich physics, such as the random-singlet (RS) phase for spin- $\frac{1}{2}$ chains.⁵⁻⁷ Recently, this technique has been extended to higher-spin cases,⁸⁻¹¹ where two of the main debates are on the robustness of the Haldane gap¹² against disorder and on the presence of the spin-1 RS phase. A number of numerical studies have also been carried out¹³⁻¹⁶ to establish a quantitative phase diagram. However, this problem has not been sufficiently clarified yet. One of the main difficulties in simulating random quantum systems is the extremely wide energy scale that has to be taken into account. Another difficulty

is the lack of appropriate physical quantity for effectively discussing randomness-driven critical behavior.

In this Letter, we report the results of our quantum Monte Carlo (QMC) simulation on the bond-alternating Haldane chain with bond randomness. By using the recently proposed twist order parameter¹⁷ together with a novel numerical technique for simulating the ground state in the framework of the loop cluster QMC method,¹⁸⁻²⁰ we show that the difficulties mentioned above can be overcome. Thus, we successfully establish the quantitative ground-state phase diagram.

We start with the following Hamiltonian for the AF Heisenberg chain

$$\mathcal{H} = \sum_{j=1}^L J_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}. \quad (1)$$

Here, \mathbf{S}_j is the spin-1 operator at site j and L the system size; periodic boundary conditions are imposed.

For the bond-alternating model without disorder, where the coupling constants $\{J_j\}$ are given by $J_j = 1 - (-1)^j \delta$ parameterized by the strength of bond alternation δ , its ground state has been discussed in terms of the valence-bond solid (VBS) picture.²¹ For the spin size S , the pattern of the valence bonds (m, n) , where m ($n = 2S - m$) denotes the number of effective singlet pairs on odd (even) bonds, changes from $(0, 2S)$ to $(2S, 0)$ successively as δ is increased from -1 to 1 , indicating the existence of $2S$ quantum phase transitions.²² Each VBS state has a topological hidden order, which is characterized by the string order parameter.²³

On the other hand, Affleck and Lieb studied Haldane's conjecture on the basis of the Lieb-Schultz-Mattis (LSM) argument.²⁴ Although the association between the VBS picture and the LSM argument has not been fully understood for a long time, Nakamura and Todo have recently shown that the ground-state expected value of the unitary operator appearing in the LSM argument, given by

$$z_L = \langle \exp[i \frac{2\pi}{L} \sum_{j=1}^L j S_j^z] \rangle, \quad (2)$$

*Present address: Speech Interface Technology Group, NEC Corporation, Kawasaki 211-8666, Japan.

†E-mail address: wistaria@ap.t.u-tokyo.ac.jp

functions as an order parameter, which characterizes the VBS states.¹⁷ The unitary operator in eq. (2) rotates the spins about the z -axis with the relative rotation angle $2\pi/L$; thus, it generates a low-lying excited state with an excitation energy of $\mathcal{O}(L^{-1})$. Since the twist order parameter (2) measures the overlap between the ground state and such a twisted excited state, $|z_L| \neq 1$ in the thermodynamic limit evidences the existence of gapless low-lying excitations or a degeneracy in the ground state. Furthermore, it is shown that in the (m, n) VBS phase, z_L converges to $(-1)^m$ for $L \rightarrow \infty$. We will see below that the twist order parameter works fairly well even in the presence of disorder.

In what follows, we consider two different random distributions for the couplings $\{J_j\}$ in eq. (1). The first one is the *uniform distribution*, where the coupling constants are distributed uniformly according to

$$P(J_j) = \begin{cases} 1/2W & \text{if } |J_j - 1 + (-1)^j \delta| \leq W \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

Here $0 \leq W \leq 1 - |\delta|$ must be fulfilled, otherwise ferromagnetic bonds could appear in the system. The second distribution is given by

$$J_j = [1 - (-1)^j \delta] t_j \quad (4)$$

with the quenched random numbers t_j obeying the *power-law distribution*^{5, 6, 25}

$$P(t_j) = \begin{cases} R^{-1} t_j^{-1+1/R} & \text{if } 0 < t_j \leq 1 \\ 0 & \text{otherwise,} \end{cases} \quad (5)$$

with a non-negative parameter R , where the $R \rightarrow 0$ limit corresponds to the nonrandom case ($t_j = 1$ for all j). Note that at $\delta = 0$ the uniform distribution (3) with $W = 1$ is equivalent to the power-law distribution [eqs. (4) and (5)] with $R = 1$ besides a trivial scaling factor; J_j 's are distributed uniformly between 0 and a finite cutoff. In the following simulations, we take the random average over 1000 samples for each parameter set.

The present model (1) can be simulated efficiently by the loop cluster QMC method^{18, 19} even in the presence of randomness. However, it should be pointed out that the loop cluster method, which is based on the Suzuki-Trotter path-integral representation, works indeed at a finite temperature. Since the ground-state properties are only our main concern in the present study, an effective extrapolation scheme, which we will explain below, for taking the zero-temperature limit is essential.

We notice the fact that the ground state of the nearest-neighbor AF Heisenberg chain of finite and even number of spins is singlet, and there is a finite gap above the ground state. In the path-integral representation, the inverse of the gap is given by the correlation length along the imaginary-time axis. Since loop size is directly related to the correlation length in real space as well as in the imaginary-time direction,^{18, 19} the system cannot distinguish whether the temperature is finite or zero, if no loops wrap around the lattice in the imaginary-time direction. In other words, the winding number of the loops in the imaginary-time direction can be used as a good measure of the convergence to the ground state.

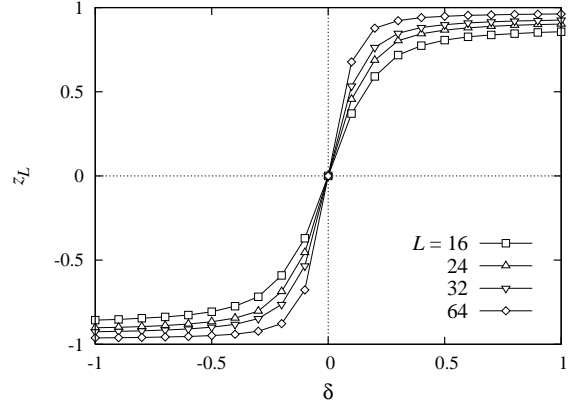


Fig. 1. δ -dependence of twist order parameter z_L for spin- $\frac{1}{2}$ system with $R = 0.5$. At $\delta = 0$, z_L is zero irrespective of system size, while it converges to ± 1 for $\delta \neq 0$.

Although there exist several means of implementing the above idea as a ground-state QMC algorithm,^{20, 26} we employ the following in the present study. We start with a certain temperature. During the thermalization Monte Carlo sweeps, the winding number of the loops is monitored. If one or more loops wrap around the system in the imaginary-time direction, we double the inverse temperature. This procedure will automatically adjust the simulation temperature so that the system will be at the ground state effectively.

Before jumping to the spin-1 system, we discuss briefly the phase diagram of the spin- $\frac{1}{2}$ system, for which the effects of disorder on this system have been well established. The ground state of the non-bond-alternating spin- $\frac{1}{2}$ chain without disorder is critical. By introducing infinitesimal randomness, the system is driven to the RS phase, where there is also no excitation gap, but the correlation function decays with an exponent different from that of the nonrandom system.⁶ The RS phase is characterized by an infinite dynamical exponent, i.e., a logarithmic scaling of the length and energy scales. As a result, the uniform susceptibility diverges as $\chi \sim 1/T \log^2 T$ at low temperatures.²⁷

The RS phase is unstable against bond alternation. The real-space correlation becomes short-ranged immediately, though the spin gap remains absent up to a finite strength of bond alternation.^{7, 27} This phase is referred to as the quantum Griffiths (QG) phase, where the uniform susceptibility obeys the power law ($\chi \sim T^{-\gamma}$) at low temperatures with a nonuniversal exponent γ varying with δ .

In Fig. 1, the twist order parameter is plotted as a function of δ for the spin- $\frac{1}{2}$ chain with $R = 0.5$ (power-law distribution). The twist order parameters with different system sizes clearly cross at $\delta = 0$. Note that in the random system, the translational and parity symmetries are both broken in each sample, and thus z_L does not necessarily become zero at $\delta = 0$. However, one sees in Fig. 1 that the symmetries are restored after the random average is taken. For a nonzero δ , the twist order parameter rapidly converges to ± 1 , though gapless QG phases extend on the both sides of the RS point.^{7, 27} The present results demonstrate clearly that the twist order

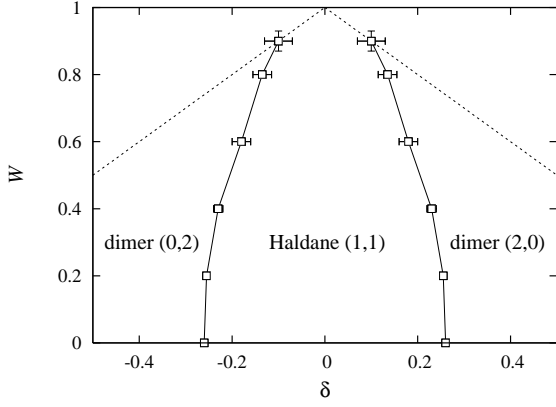


Fig. 2. Ground-state phase diagram of spin-1 chain with uniform random-bond distribution. Along the $\delta = 0$ line, the Haldane phase survives up to $W = 1$.

parameter z_L is not affected by QG singularity, and thus it is an effective tool for analyzing RS criticality.

In contrast to the spin- $\frac{1}{2}$ chain, the non-bond-alternating spin-1 Haldane system without disorder has a finite gap and a finite correlation length.¹² In the previous DRG studies,^{8,9} it is predicted that the Haldane state is stable against a weak disorder, while there occurs a quantum phase transition to the spin-1 RS phase at a critical strength of randomness. In the previous QMC analysis¹⁵ of the model with a uniform random-bond distribution (3), in which the uniform susceptibility and the string order parameter were mainly investigated along the $\delta = 0$ line, it was concluded that a quantum phase transition occurs at $W \simeq 0.95$ from the Haldane phase to the RS phase. In the present calculation, however, the twist order parameter decreases with increasing system size in the entire range of W ($0 \leq W \leq 1$), and tends to converge to -1 without showing any crossing, which indicates that the Haldane [(1,1) VBS] phase is stable in the entire range of W .

This can be seen more clearly in the δ - W phase diagram shown in Fig. 2. The phase boundaries are obtained from the crossing point of the twist order parameter with different system sizes ($L = 8 \cdots 64$). For small δ 's, where the Haldane phase existing at $|\delta| < 0.25997(3)$ for $W = 0$ ¹⁷ decreases gradually, the phase diagram [Fig. 2] agrees qualitatively with the one predicted by the DRG analysis.¹⁰ However, the phase boundary between the Haldane (1,1) and the dimer (2,0) phases (solid line) merges with the parameter boundary $\delta + W = 1$ (dashed line) at $\delta \simeq 0.1$, and does *not* reach $\delta = 0$ even at $W = 1$, indicating that there is no spin-1 RS phase in the model with the uniform random-bond distribution.

Next, we examine the other random-bond distribution, i.e., the power-law distribution [eqs. (4) and (5)]. As already mentioned, the power-law distribution with $R = 1$ is equivalent to the uniform one with $W = 1$; thus, it is expected that the Haldane phase is stable at least up to $R = 1$ also for the former case. However, for the power-law distribution, one can consider a further strong disorder ($R > 1$), i.e., a wider distribution on the logarithmic scale, by which the Haldane phase might be broken.²⁵

In the inset of Fig. 3, the twist order parameter is plot-

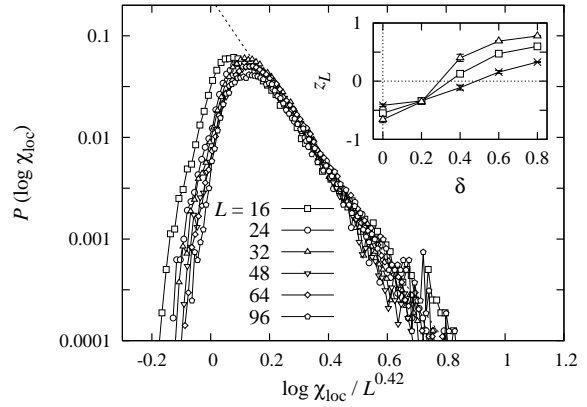


Fig. 3. Scaling plot of distribution function of local susceptibility at RS point $(R, \delta) = (0.5, 0.2)$. Inset: δ -dependence of twist order parameter for $R = 0.5$ (crosses, squares, and triangles for $L = 8, 16$ and 32 , respectively.)

ted as a function of δ in the weak randomness regime ($R = 0.5$). For $\delta > 0.2$, the twist order parameter increases as the system size increases and tends to converge to +1. We identify this phase as the dimer (2,0) phase. On the other hand, z_L tends to converge to -1 for $\delta < 0.2$, indicating the Haldane (1,1) phase.

At the crossing point $\delta = 0.20(1)$, a quantum phase transition occurs, and the transition is expected to belong to the spin- $\frac{1}{2}$ RS universality class.¹⁰ To confirm this prediction, we measured the distribution of the local susceptibility

$$\chi_{\text{loc},j} = \beta \langle m_j^2 \rangle = \int_0^\beta d\tau \langle S_j^z(0) S_j^z(\tau) \rangle \quad (6)$$

at the critical point $(R, \delta) = (0.5, 0.2)$. As seen in Fig. 3, the distribution function of the logarithm of the local susceptibility is scaled fairly well by assuming a logarithmic scaling form, $P(\log \chi_{\text{loc}}) \simeq \tilde{f}(\log \chi_{\text{loc}} / L^\psi)$ with $\psi = 0.42$. This is consistent with the previous DRG prediction for the RS phase,⁶ though the exponent ψ is slightly smaller than the predicted value ($\psi = 1/2$). This is additional support to the validity of applying the twist order parameter to randomness-driven quantum phase transitions. Repeating similar analyses, we obtain the entire δ - R phase diagram of the random Haldane chain with the power-law distribution [Fig. 4].

Although the phase diagram for the power-law distribution is similar to Fig. 2 for small R 's, the overall shape of the phase boundaries indicates the existence of a multicritical point, where two critical lines merge with each other at a finite R . To locate the multicritical point, we calculate z_L for several system sizes ($L = 16 \cdots 64$) along the $\delta = 0$ line. The results for $0.9 \leq R \leq 1.2$ is shown in Fig. 5, where the data with different system sizes clearly cross at $R_c \simeq 1.05$. Thus, we conclude that there exists a multicritical point at $(R, \delta) = (1.05, 0)$, which is indicated by the solid square in Fig. 4. Below the multicritical point, the Haldane phase survives, though the spin gap vanishes at a certain R ($< R_c$), where a crossover from the gapped Haldane phase to the gapless Haldane (or QG) phase occurs. In the case of a uniform distribution (3), the crossover is observed at $W \simeq 0.7$,²⁷ though

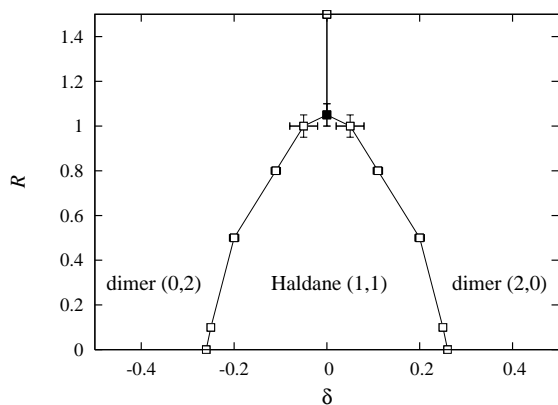


Fig. 4. Ground-state phase diagram of spin-1 chain with power-law random-bond distribution. The multicritical point is indicated by the filled square.

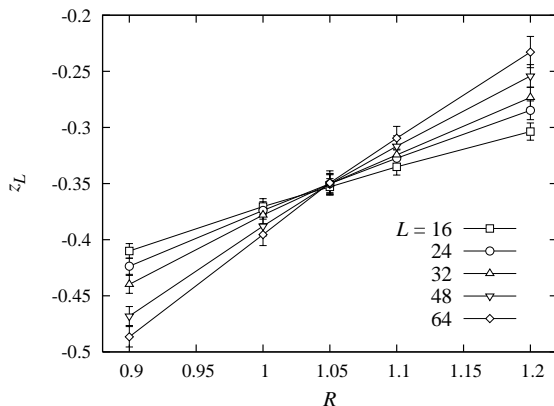


Fig. 5. R -dependence of twist order parameter z_L of spin-1 system with $\delta = 0$. The data with different system sizes cross at $R \simeq 1.05$.

we have not yet examined it for the power-law distribution. For $R > R_c$, on the other hand, the twist order parameter is expected to converge to a nontrivial value (i.e., $z_L \neq \pm 1$) in the thermodynamic limit, where the spin-1 RS phase is realized.^{8–10}

To summarize, we reported the results of our QMC simulations on the bond-alternating random Haldane chain. By introducing the ground-state loop cluster QMC method and the twist order parameter, we have successfully calculated the ground-state phase diagram. In particular, we demonstrated that the twist order parameter, introduced originally for pure spin chains, is also effective for random spin chains. Indeed, it is shown that the behavior of the twist order parameter observed in the present study can be discussed more directly in terms of the numerical DRG approach, in which one can calculate the topological order parameter for an approximate VBS-like ground state explicitly.²⁸

For the uniform distribution, the present result, i.e., the absence of the spin-1 RS phase, does not agree with the previous finite-temperature QMC result, in which a multicritical point was suggested.¹⁵ The possible reason for this disagreement is that the finite-temperature QMC method might easily fail to take into account rare

and low-energy-scale but very strong correlations, which are essential in random spin systems. In contrast, in the present ground-state algorithm, simulation temperature is automatically adjusted according to the magnitude of the gap of each random sample, so that the physical quantity at the zero temperature is calculated at an optimal cost. This algorithm is useful in simulating not only random systems but also those without disorder.²⁰

For the power-law distribution, on the other hand, we established a phase diagram with a multicritical point, whose location was also determined accurately using the twist order parameter. The present phase diagram agrees qualitatively with the recent DRG prediction,¹⁰ though the numerical confirmation of spin-1 RS criticality, which is expected to realize in the strong disorder regime ($R > R_c$), still remains as a future problem.

We acknowledge our fruitful discussion with M. Nakamura. The simulations presented in this Letter have been performed using the facility of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo. S.T. acknowledges the support by a Grant-in-Aid for the Scientific Research Program (No.15740232) from the Japan Society for the Promotion of Science.

- 1) M. Matsumoto, C. Yasuda, S. Todo and H. Takayama: Phys. Rev. B **65** (2002) 014407.
- 2) M. Hase, N. Koide, K. Manabe, Y. Sasago, K. Uchinokura and A. Sawa: Physica B **215** (1995) 164.
- 3) C. Yasuda, S. Todo, M. Matsumoto and H. Takayama: Phys. Rev. B **64** (2001) 092405.
- 4) C. Yasuda, S. Todo, M. Matsumoto and H. Takayama: J. Phys. Chem. of Solids **63** (2002) 1607.
- 5) C. Dasgupta and S. K. Ma: Phys. rev. B **22** (1980) 1305.
- 6) D. S. Fisher: Phys. Rev. B **50** (1994) 3799.
- 7) R. A. Hyman, K. Yang, R. N. Bhatt and S. M. Girvin: Phys. Rev. Lett. **76** (1996) 839.
- 8) R. A. Hyman and K. Yang: Phys. Rev. Lett. **78** (1997) 1783.
- 9) C. Monthus, O. Golinelli and Th. Jolicœur: Phys. Rev. Lett. **79** (1997) 3254.
- 10) K. Damle: Phys. Rev. B **66** (2002) 104425.
- 11) A. Saguia, B. Boechat and M. A. Continentino: Phys. Rev. Lett. **89** (2002) 117202.
- 12) F. D. M. Haldane: Phys. Lett. **93A** (1983) 464; Phys. Rev. Lett. **50** (1993) 1153.
- 13) Y. Nishiyama: Physica A **252** (1998) 35.
- 14) K. Hida: Phys. Rev. Lett. **83** (1999) 3297.
- 15) S. Todo, K. Kato and H. Takayama: J. Phys. Soc. Jpn. Suppl. A **69** (2000) 355.
- 16) E. Carlon, P. Lajkó, H. Rieger and F. Iglói: Phys. Rev. B **69** (2004) 144416.
- 17) M. Nakamura and S. Todo: Phys. Rev. Lett. **89** (2002) 077204.
- 18) H. G. Evertz: Adv. Phys. **52** (2003) 1.
- 19) S. Todo and K. Kato: Phys. Rev. Lett. **87** (2001) 047203.
- 20) S. Todo: unpublished.
- 21) I. Affleck, T. Kennedy, E. Lieb and H. Tasaki: Phys. Rev. Lett. **59** (1987) 799.
- 22) M. Oshikawa: J. Phys. Condens. Matter **4** (1992) 7469.
- 23) M. den Nijs and K. Rommelse: Phys. Rev. B **40** (1989) 4709.
- 24) I. Affleck and E. Lieb: Lett. Math. Phys. **12** (1986) 57.
- 25) K. Yang and R. A. Hyman: Phys. Rev. Lett. **84** (2000) 2044.
- 26) H. G. Evertz and W. von der Linden: Phys. Rev. Lett. **86** (2001) 5164.
- 27) S. Todo, K. Kato and H. Takayama: *Computer Simulation Studies in Condensed-Matter Physics XI*, ed. D. P. Landau and H.-B. Schüttler (Springer, Berlin, Heidelberg, 1999) p. 57.
- 28) S. Todo, T. Arakawa and H. Takayama: unpublished.